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GUMRAP
A Computer Program for Analyzing Molecular Flow in Complex Enclosures

Max Kinslow
ARO, Inc.

February 1980

Final Report for Period October 1, 1978 – September 24, 1979

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The General Unwanted Energy Rejection Analysis Program (GUERAP), which uses a Monte Carlo ray trace technique to analyze complex optical systems, has been in use for a number of years. This report describes the development of a molecular ray trace computer code (GUMRAP) based upon the extensive geometric and Monte Carlo ray trace portion of GUERAP. Portions of GUERAP strictly concerned with radiation such as diffraction, refraction, and internal radiation

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have been removed, and a new gas-surface interaction subroutine, REFLCT, based upon the reciprocity relation, has been included. A detailed description of the input variables is given, as is a listing of control cards so that GUMRAP can be run on an IBM 370/165 computer by anyone desiring to analyze the molecular flow in complex systems such as space chambers.

AFSC
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PREFACE

The work reported herein was conducted by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC). The results of the research were obtained by ARO, Inc. (a Sverdrup Corporation Company), AEDC Division, operating contractor for the AEDC, AFSC, Arnold Air Force Station, Tennessee, under ARO Project Number V32K-15. Mr. Marshall Kingery, AEDC/DOT, was the Air Force project manager. The manuscript was submitted for publication on September 24, 1979.

CONTENTS

ILLUSTRATIONS

Figure Page

TABLES

APPENDIXES

1.0 INTRODUCTION

There is a continuing need to analyze the molecular flow in space chambers, through baffles, in ducting, and in similar complex systems. When chemical or ion rockets are tested under high altitude space conditions, it is desirable to minimize the pressure or backflow in certain regions of the test chamber. Because of the high velocity of molecules emerging from a rocket exhaust and the fact that these molecules are not immediately accommodated to chamber conditions, a systematic, analytic approach to the pretest chamber configuration optimization is desirable.

The General Unwanted Energy Rejection Analysis Program (GUERAP) has been used extensively in the past few years to analyze a variety of optical systems. GUERAP (Ref. 1) uses a Monte Carlo ray trace technique to analyze the radiation characteristics of complex optical systems.

There are many similarities between radiation ray trace and molecular ray trace techniques. It was decided that the most expeditious approach to providing the molecular flow-field analysis would be to utilize the geometric and ray trace portion of GUERAP. This modified GUERAP program is called the General Unwanted Molecule Rejection Analysis Program (GUMRAP).

The major modification to GUERAP was the elimination of several unnecessary radiation subroutines and the addition of a gas-surface interaction model. Shown below are the changes made in GUERAP.

1. Removal of diffraction of rays
2. Removal of refraction regions
3. Removal of the important surface technique
4. Removal of internal radiation
5. Removal of irrelevant radiation scattering
6. Addition of realistic gas-surface interactions model

Time limitations precluded the elimination of all FORTRAN statements and variables that are remnants from GUERAP.

2.0 GAS-SURFACE INTERACTION MODEL

It has been 100 years since Maxwell proposed that when a gas reflects from a solid surface a certain fraction of the molecules is reflected diffusely (fully accommodated) and the remainder of the molecules are reflected specularly (no accommodation). Over the years other investigators such as Nocilla (Ref. 2) and Epstein (Ref. 3) have proposed more realistic gas-surface interaction models. However, all previous models, while being more or less successful in explaining energy exchange with a surface, failed to realistically describe the scattering of individual molecules.

More recently, Cercignani (Ref. 4), Kuscer et al. (Ref. 5), and Wenaas (Ref. 6) have shown that any gas-surface interaction model, in addition to satisfying the obvious condition of maintaining the equilibrium velocity distribution at the surface temperature, must satisfy the reciprocity relation. The introduction of a scattering kernel, $P(\vec{v}',\vec{v})$, which gives the reflected probability density as a function only of incident and reflected velocity vectors, implicitly assumes that a molecule interacts with the wall on an individual basis, independent of other molecules. In other words, a molecule with velocity "v" does not "know" whether it is a rocket exhaust or part of a gas in equilibrium with the wall. This result permits the reciprocity condition on the scattering kernel, which was derived for equilibrium conditions, to be applied for nonequilibrium conditions.

2.1 BASIC EQUATIONS

The time-independent interactions between a gas and a surface may be expressed mathematically by means of a scattering kernel, $P(\vec{v}',\vec{v})$, which relates the probability that a molecule with velocity $\vec{v}'$ will be scattered by a surface into a velocity close to $\vec{v}$ (refer to Fig. 1).

Kuscer et al. (Ref. 5) point out the importance of reciprocity in connection with a mathematical description of gas-surface interaction. The reciprocity relation which must be satisfied by any scattering kernel is

$$-v_y' P(\vec{v}',\vec{v}) \exp\left(-\vec{v}'^2/2RT_w\right) = v_y P(-\vec{v},-\vec{v}') \exp\left(-\vec{v}^2/2RT_w\right) \tag{1}$$

In addition, $P(\vec{v}', \vec{v})$ must satisfy the obvious condition of being non-negative and, for no mass exchange with the surface, normalized in half velocity space. In other words,

$$P(\vec{v}',\vec{v}) \geq 0 \text{ for } \begin{matrix} v_y' \leq 0 \\ v_y \geq 0 \end{matrix} \tag{2}$$

and

$$\int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{-\infty}^{\infty} P(\vec{v}',\vec{v})\, dv_x\, dv_y\, dv_z = 1 \tag{3}$$

Equation (3) states the conversation property of molecules, i.e., that molecules are assumed not to be trapped or cryopumped by a surface.

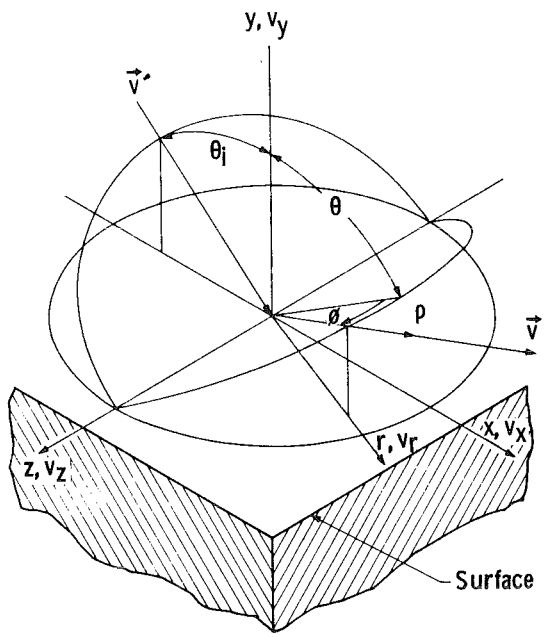


Figure 1. Coordinate systems for gas-surface interaction.

Kinslow (Ref. 7) has developed a product expression for $P(\vec{v}', \vec{v})$ that satisfies the conditions expressed in Eqs. (1), (2), and (3) and also contains the experimentally observed characteristics of gas-surface interactions as discussed in Refs. 7, 8, and 9.

The scattering kernel presented in Ref. 7 is as follows:

$$P(\vec{v}',\vec{v}) = \frac{2A_y^2 A_x A_z}{(2RT_w)^{3/2}} S_y I_o(-2A_y \sqrt{A_y^2 - 1}\, S_y' S_y)$$

$$\exp\left[-\left(\sqrt{A_x^2 - 1}\, S_x' - A_x S_x\right)^2 - (A_y^2 - 1) S_y'^2 - A_y^2 S_y^2 - \left(\sqrt{A_z^2 - 1}\, S_z' - A_z S_z\right)^2\right] \tag{4}$$

where A_x, A_y, and A_z are arbitrary constants greater than 1 and are related to the gas-surface energy accommodation coefficient, α, by

$$A_x^{-2} = \alpha_x, A_y^{-2} = \alpha_y, \text{ etc.} \tag{5}$$

For the special condition of $\alpha_x = \alpha_y = \alpha_z = 1$ (fully accommodated), Eq. (4) reduces to a fully accommodated Maxwellian velocity distribution at the surface temperature, with a cosine spatial reflection. For the condition of $\alpha_x = \alpha_y = \alpha_z = 0$ (no accommodation), Eq. (5) gives specular reflection. These correct limits help support the validity of the scattering kernel as given by Eq. (4).

In Refs. 8 and 9 it is shown that the result for the scattering kernel as given in Eq. (4) is adequate to describe existing experimental results provided appropriate A_x, A_y, and A_z where are chosen. The coordinate results from Eq. (4) in dimensionless form are as follows:

$$P_x = (\pi)^{-1/2} \exp\left[-(T_x - R_x)^2\right] \tag{6}$$

where

$$R_x = \sqrt{A_x^2 - 1}\, S_x'$$

$$T_x = A_x S_x$$

and

$$P_y = 2T_y \frac{I_o(-2R_y T_y)}{\exp(-2R_y T_y)} \exp\left[-(R_y + T_y)^2\right] \tag{7}$$

where

$$R_y = \sqrt{A_y^2 - 1}\, S'$$

$$Ty = A_y S_y$$

The term P_z can also be expressed by Eq. (6), with the x's replaced by z's.

2.2 MONTE CARLO SOLUTION OF $P(\vec{v}', \vec{v})$

Physically Eqs. (6) and (7) give the probability that a molecule with velocity components v_x', v_y', and v_z' will be reflected from a surface with velocity components v_x, v_y, and v_z. Using

the Monte Carlo solution there are two methods that can be used to determine the reflected velocities from Eqs. (6) and (7). One of these is the rejection technique, and the other is the direct, or inversion, method. For a brief description of these methods see Ref. 10.

The rejection technique is used frequently when involved mathematical equations are necessary for the evaluation of inverse probability functions. Equation (6) and especially Eq. (7), which includes the Bessel function, I_o, are time-consuming to evaluate. Since the Monte Carlo method requires many samples to give meaningful results, the evaluation of any involved numerical scheme should be avoided. It was therefore decided to use the direct method with a numerical approximation to the inverse scattering kernel, as follows.

Define functions Q_x and Q_y as

$$Q_x(T_x) = \int_{-\infty}^{T_x} P_x \, dT_x \tag{8}$$

and

$$Q_y(T_y) = \int_{0}^{T_y} P_y \, dT_y \tag{9}$$

Since P_x and P_y are normalized, the values of Q_x and Q_y vary from zero to unity. It can be shown that the probability density of Q_x and Q_y is unity; in other words, for a given S_x' and S_y' any Q_x or Q_y between zero and one is equally probable. This fact is the basis of the direct selection technique. By obtaining a random number between zero and one and equating that to Q, one can solve Eq. (8) or (9) for T and thus find the reflected velocity components from the definitions of T_x, T_y, S_x, and S_y.

As stated above, a curve fit to Eqs. (6) through (9) will be used. Given Q and R, the problem is to find T and therefore v_x, v_y, and v_z. It is desirable to use a linear approximation, and it was found that by redefining variables a suitable form was obtained. For example, R can vary over all values, and the curves are asymptotic with R as a parameter; however, if one uses $R^2/(0.5 + R^2)$ as a parameter, whose value is between zero and unity, the curves are more linear. The other parameter used, which also has limited variation, was

$$T - R^2 \; / \; (0.5 + R)$$

From the asymptotic expansion of the Bessel function, I_o, it can be shown that as $(2 R_y) \rightarrow \infty$, Eq. (7) reduces to Eq. (6). This fact is used to permit 1) use of the results for

Eqs. (7) and (9) and 2) inclusion of the results for the x and z components as given by Eqs. (6) and (8).

Based upon the results of the reciprocity relation and the numerical curve fitting described above, a computer subroutine was written to calculate the reflection from a surface. This subroutine, REFLCT, is given in Appendix A.

2.3 NUMERICAL RESULTS FROM GAS-SURFACE MODEL

In order to check the reciprocity gas-surface model and its implementation in REFLCT and also to gain insight into the characteristics of reflected molecular properties, a simple parametric analysis was performed. Assuming a molecular beam of argon with normal and tangential velocity components of 10,000 ft/sec, which is a speed of 14,142 ft/sec at an incidence angle of 45 deg, the reflected properties were determined for surface temperatures, T_s, of 300 and 30°K and also for energy accommodation coefficients, α, of 0.9 and 0.5. Since multiple encounters of molecules with the surface are important in the accommodation to space chamber conditions, each molecule was allowed to undergo 10 collisions with the test surface. A total of 100,000 molecules was followed for the 10 surface interactions; thus 1,000,000 gas-surface encounters were calculated using the Monte Carlo technique for each condition.

In a real enclosure the number of encounters a molecule will have with surfaces can vary from zero to an unlimited number. After a molecule enters the enclosure through an entrance area, it is followed as it makes encounters with various surfaces until it is captured by a surface (i.e., cryopumped) or leaves the enclosure through the exit or entrance. Also, tracking of the molecule can be stopped after a number of surface collisions, which can be input into the program. However, in the present example no surface capture takes place, and no molecules can exit. The number of surface encounters allowed (10) is completely arbitrary.

For an isothermal enclosure, molecules, independent of their initial velocities, will approach, after a sufficient number of surface collisions, a Maxwellian, fully accommodated velocity distribution. Spatially, a fully accommodated distribution is equivalent to a cosine distribution.

The results of this numerical study are presented in Figs. 2 through 7 in two different ways. First, in Figs. 2 and 3 the reflected velocity distribution is shown for various values of surface collisons, N, for $\alpha = 0.5$ and 0.9 and $T_s = 30$ and 300°K. Notice that for $\alpha = 0.9$ (Fig. 3) the velocity distribution has become a fully accommodated Maxwellian distribution

at the surface temperature for 10 surface collisions. Second, in Figs. 4 through 7 the results are given as reflected spatial or angular distributions. For the case of $\alpha = 0.9$ and $N = 10$ as shown in Fig. 7 the fully accommodated cosine distribution is obtained.

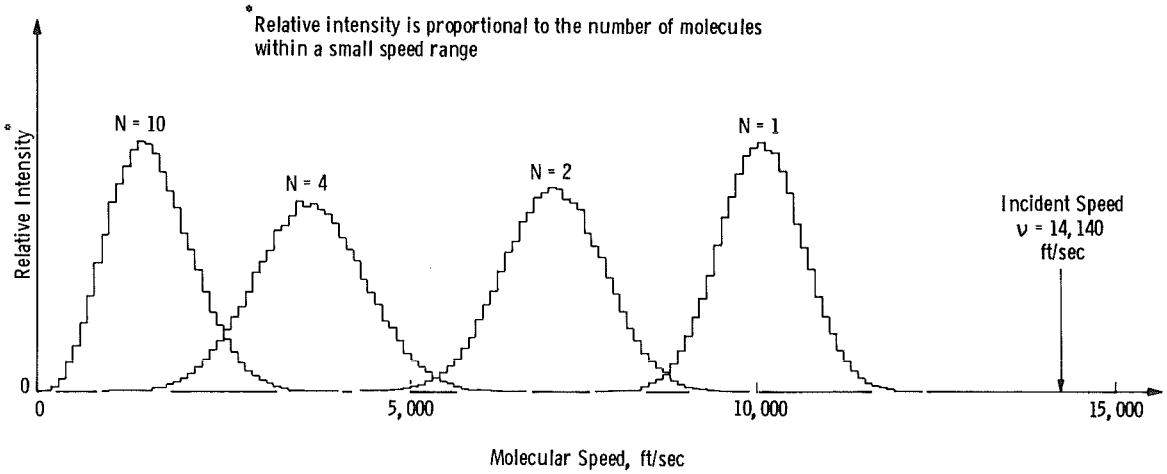


Figure 2. Reflected velocity distribution for $T_s = 300°K$ and $\alpha = 0.5$.

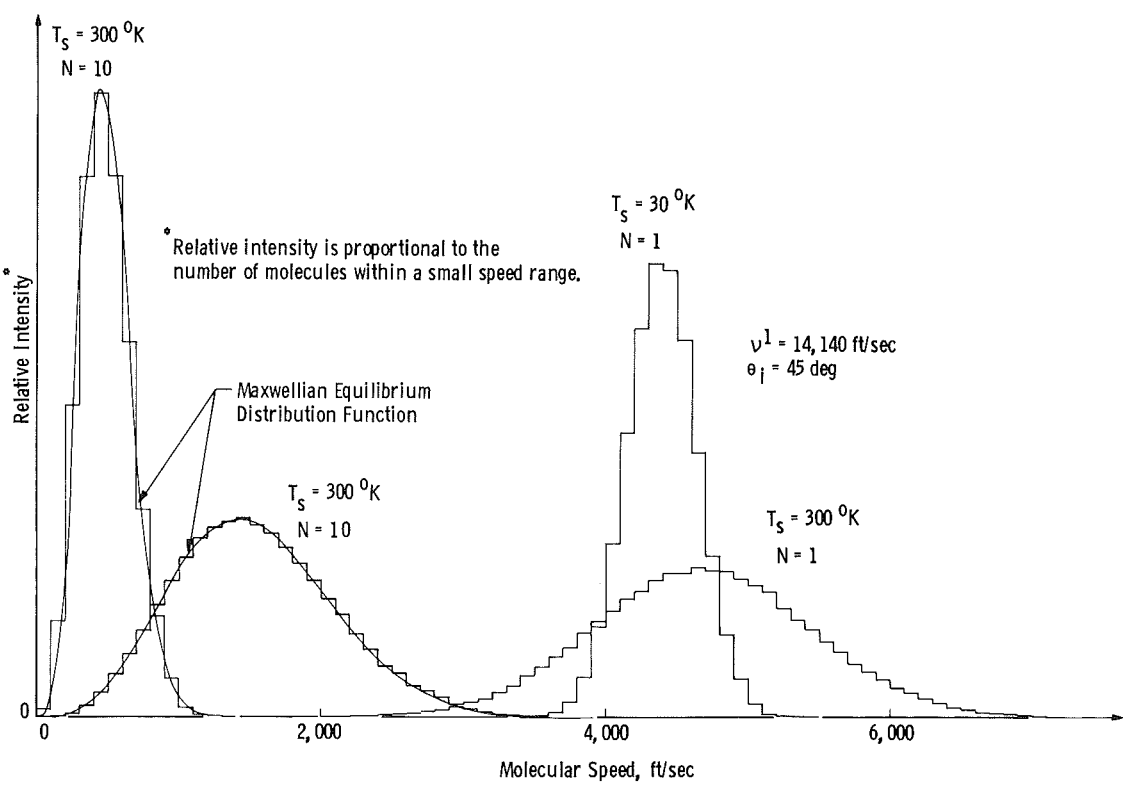
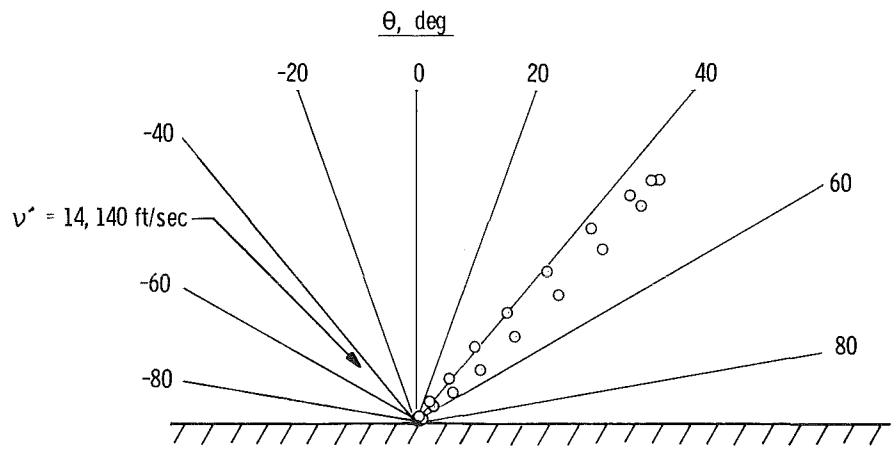
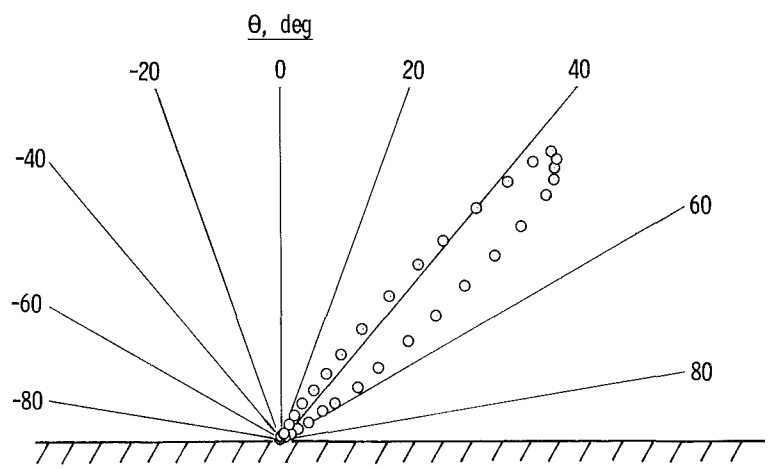


Figure 3. Effect of surface temperature, T_s, on reflected velocity distribution for $\alpha = 0.9$.

Note: Radial coordinate is proportional to the number of molecules reflected in a small solid angle.



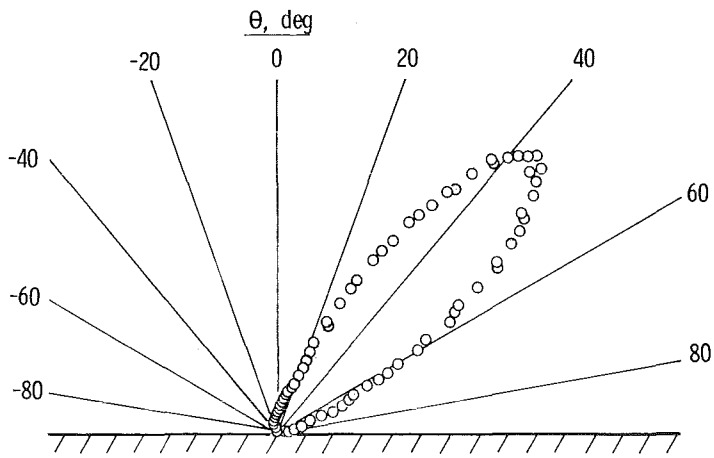
a. N = 1



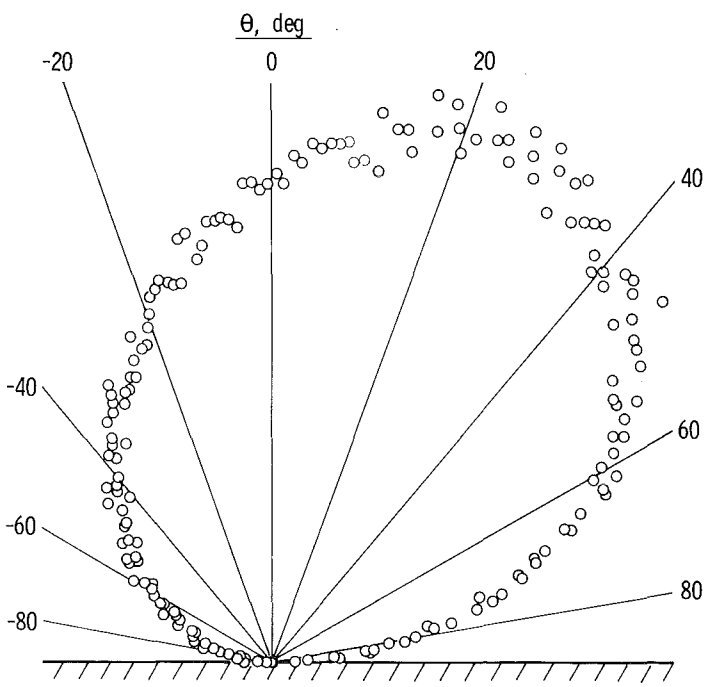
b. N = 2

Figure 4. Reflected spatial distribution for α = 0.5 and T_s = 300°K.

Note: Radial coordinate is proportional to the number of molecules reflected in a small solid angle.



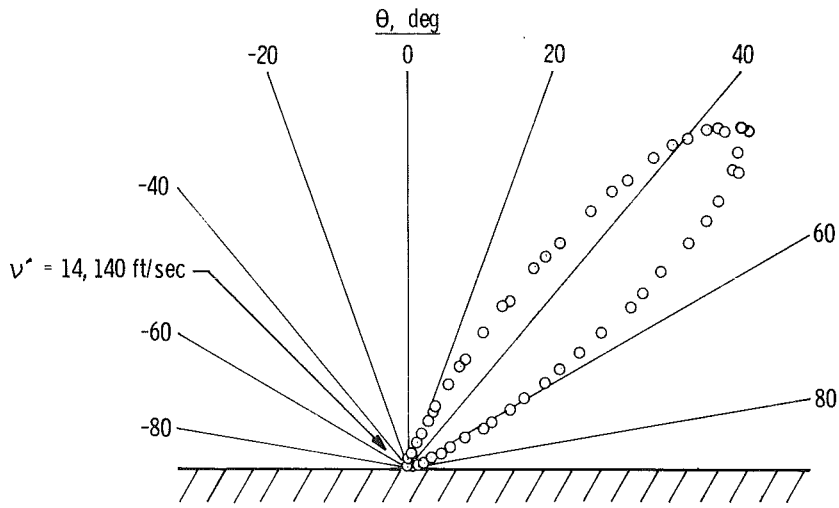
c. N = 4



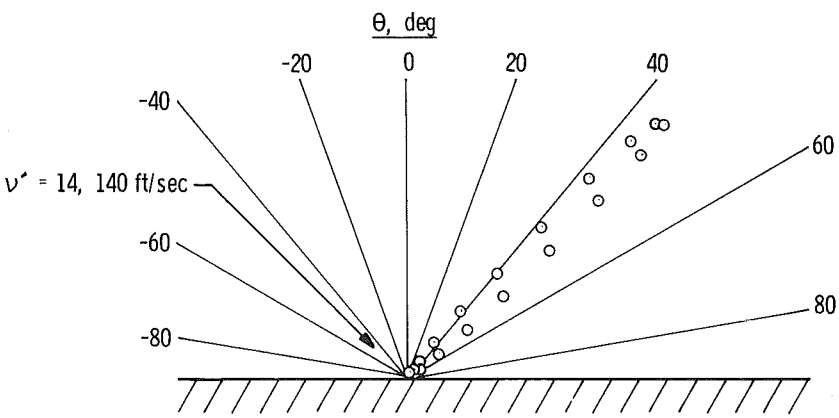
d. N = 10

Figure 4. Concluded.

Note: Radial coordinate is proportional to the number of molecules reflected in a small solid angle.



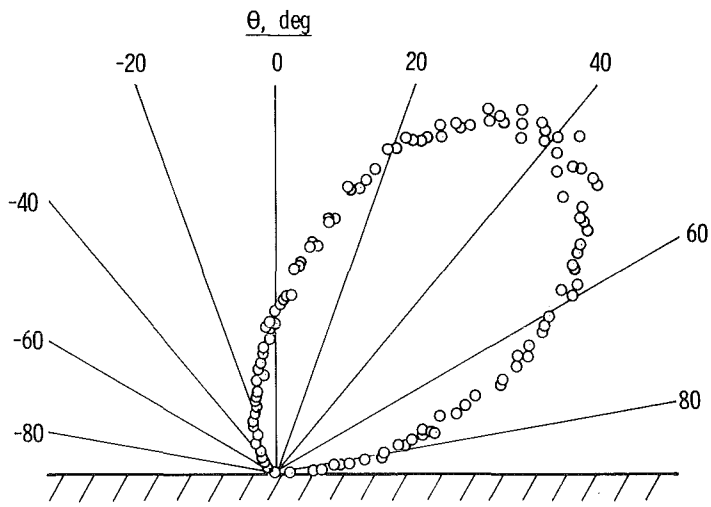
a. T_s = 300°K



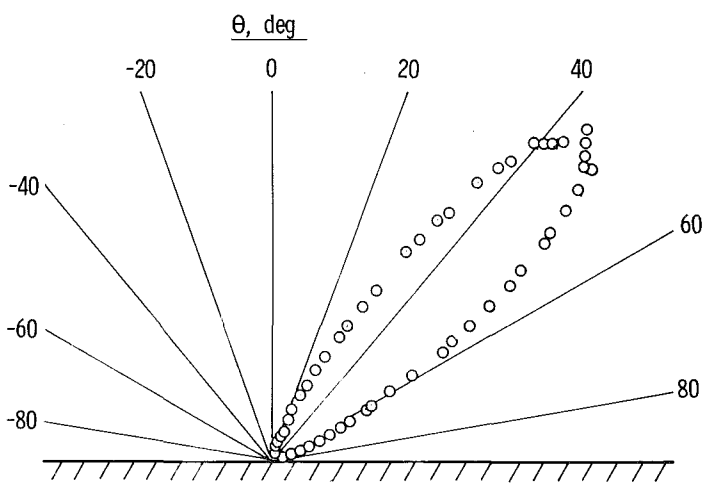
b. T_s = 30°K

Figure 5. Reflected spatial distribution for α = 0.9 and N = 1.

Note: Radial coordinate is proportional to the number of molecules reflected in a small solid angle.



a. T_s = 300°K



b. T_s = 30°K

Figure 6. Reflected spatial distribution for a = 0.9 and N = 2.

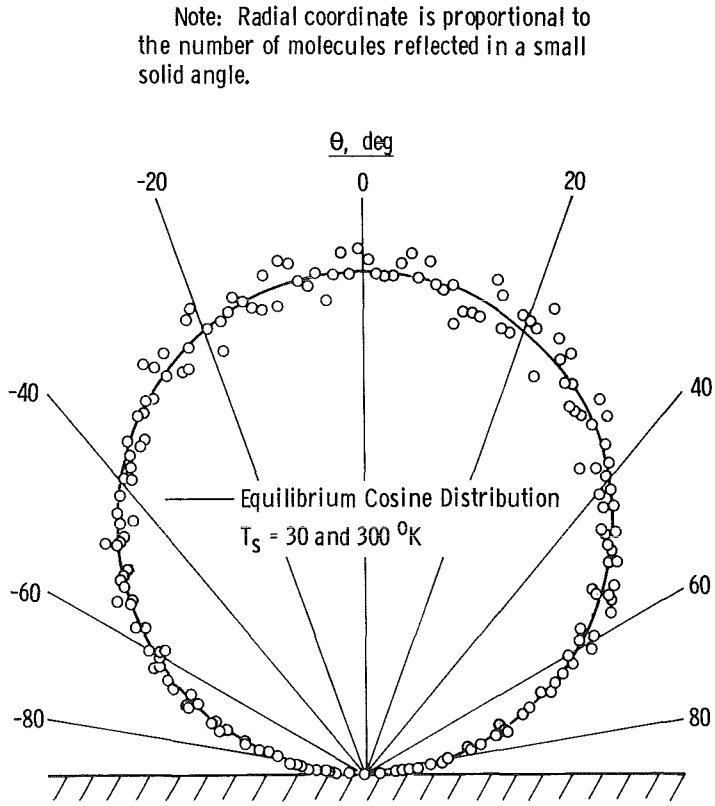


Figure 7. Reflected spatial distribution for a = 0.9 and N = 10.

One characteristic of the Monte Carlo technique evident in these calculations is the random scatter of the results. This is best seen in Fig. 7, where most of the points are within ±5 percent of the mean. It can be shown from statistical theory that the variation of a random process, such as the Monte Carlo method, about the mean is a Gaussian distribution with a width or mean error proportional to $N^{-1/2}$. Thus, in order to reduce the numerical scatter by a factor of two, four times as large a sample would be required (i.e., N = 400,000 for the present calculation).

Based upon the results of this limited analysis the following conclusions can be drawn:

1. For N = 1 the reflection is close to specular, with almost all reflected molecules having the same tangential direction as the incident beam.
2. The reflected distribution for lower surface temperature is narrower both in velocity spread and in spatial variation than that for higher surface temperature.

3. For higher accommodation coefficients the reflection is more diffuse, and equilibrium conditions are approached with fewer surface collisions than for lower values of α.

As shown in Refs. 7, 8, and 9, the reciprocity gas-surface scattering model is the only existing theory that agrees with available experimental data. In addition, the implementation of the present model in REFLCT also realistically describes the accommodation of molecules to the conditions of an enclosure.

On the basis of these facts, a duplicate of the existing GUERAP computer code was modified to eliminate thermal radiation peculiar parts and add the improved gas-surface model subroutine REFLCT. Changing the energy ray-trace technique to a molecule ray trace prompted changing the E in GUERAP to an M, giving rise to the name GUMRAP for the modified version.

No details on the changes made to GUERAP are given here. However, a detailed description of input variables required to run GUMRAP is presented.

3.0 NUMERICAL INPUTS TO GUMRAP

This section contains a detailed definition of important input variables. Appendix B lists all input parameters, a simplified description, and the default values used in the program if no overriding values are input. It is suggested that one make a sketch of the complete system and check all inputs before attempting to run the program.

There are several types of inputs to GUMRAP, including the following:

1. Geometric inputs of system configuration
2. Properties of surfaces that make up the geometric system
3. Properties of incident molecular beam in regard to molecular weight, velocity, direction, etc.
4. Input data in regard to random number generation
5. Options for printing output.

Most data are input via the namelist statment, a standard feature of FORTRAN.

3.1 GEOMETRIC INPUTS (NMGEOM)

The first namelist is called NMGEOM and inputs most of the geometry of the system. GUMRAP can analyze systems of up to 30 surfaces or boundaries. Any system can also be divided into as many as five sections. In order to simplify the geometric input, seven standard-type surfaces have been defined.

Each surface, identified by N, is assigned a number and is used to identify section boundaries, surface constraints, etc. The seven standard surface types will be described first. These seven surfaces are:

1. Plane
2. Cone
3. Sphere
4. Paraboloid
5. Ellipsoid
6. Hyperboloid
7. Baffle

The parameters for these surfaces as well as optional standard constraints are input by the FORTRAN variable array PLTCTR(11,30) where up to 11 values may be input to describe each of the up to 30 surfaces. The type of each surface is identified by a group of arrays as follows:

IPLANE(I) = NS (Surface number of I^{th} Plane)

ICONE(I) = NS (Surface number of I^{th} Cone)

ISHPER(I) = NS (Surface number of I^{th} Sphere)

IPARAB(I) = NS (Surface number of I^{th} Paraboloid)

IELPS(I) = NS (Surface number of I^{th} Ellipsoid)

IHYPB(I) = NS (Surface number of I^{th} Hyperboloid)

IBAFF(I) = NS (Surface number of I^{th} Baffle)

The inputs to PTLCTR are detailed in Table I for the seven standard surfaces. Figures 8 through 16 define the various parameters. Notice that the baffle (Figs. 15 and 16) has no outer constraint; special constraints, which will be discussed later, must be used.

Table 1. Definition of PTLCTR(J,N) Inputs

Surface	Figure Number	PTLCTR(1,N) =	Remarks
Plane (Disk)	8	X_c, Y_c, Z_c, α, β, γ, R_1, R_2	Unit Normal should point into region.
Plane (Rectangle)	9	X_1, Y_1, Z_1, α_1, β_1, γ_1, A, B, α_2, β_2, γ_2	
Cone	10	X_1, Y_1, Z_1, X_2, Y_2, Z_2, R_1, R_2	
Sphere	11	X_1, Y_1, Z_1, X_2, Y_2, Z_2, R_1, R_2	
Paraboloid	12	X_1, Y_1, Z_1, X_2, Y_2, Z_2, R_1, R_2	
Ellipsoid	13	X_1, Y_1, Z_1, X_2, Y_2, Z_2, R, R_c	
Hyperboloid	14	X_1, Y_1, Z_1, X_2, Y_2, Z_2, B, R_c	
Plane Baffle	15	X_c, Y_c, Z_c, α, β, γ, R, 0.	Also Input RKNIFE = R_e DBAFF = δ ABAFFD = ε TBAFF = t
Conical Baffle	16	X_c, Y_c, Z_c, α, β, γ, R, ψ	

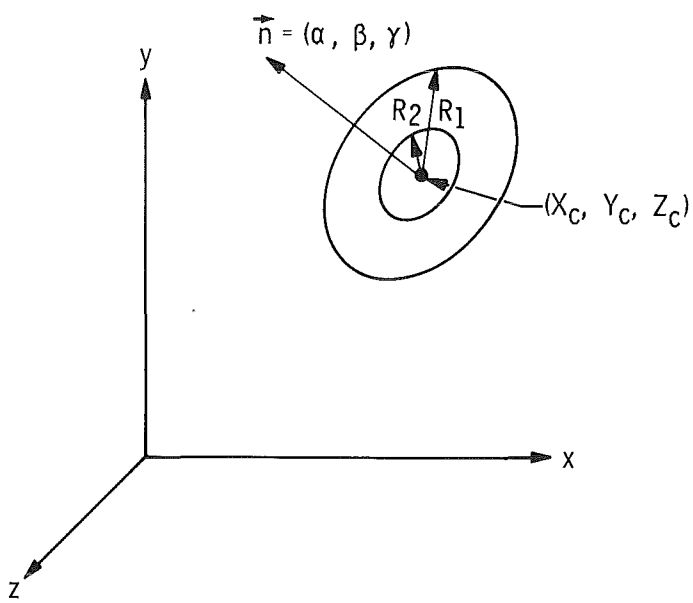


Figure 8. Plane (disk) configuration.

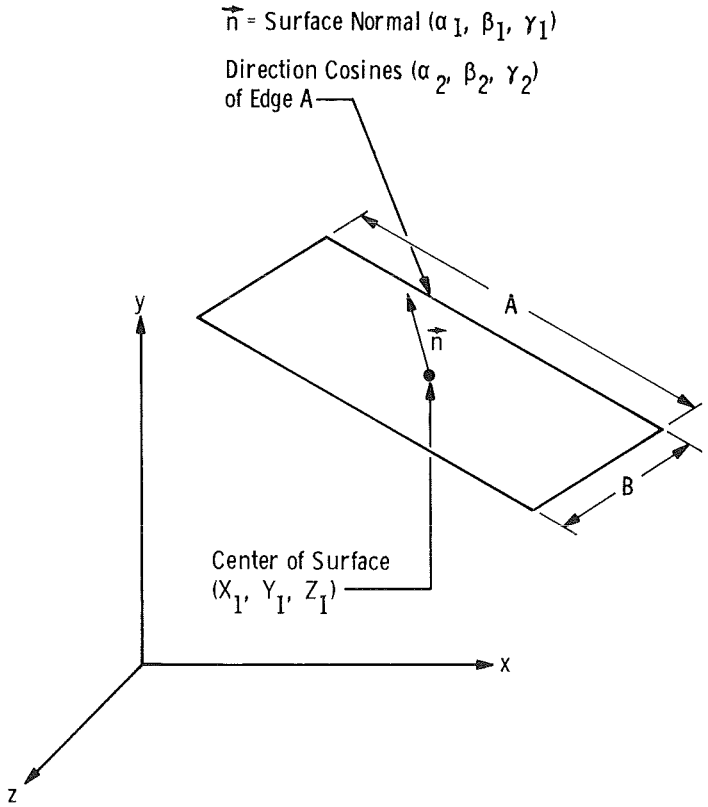


Figure 9. Plane(rectangle) configuration.

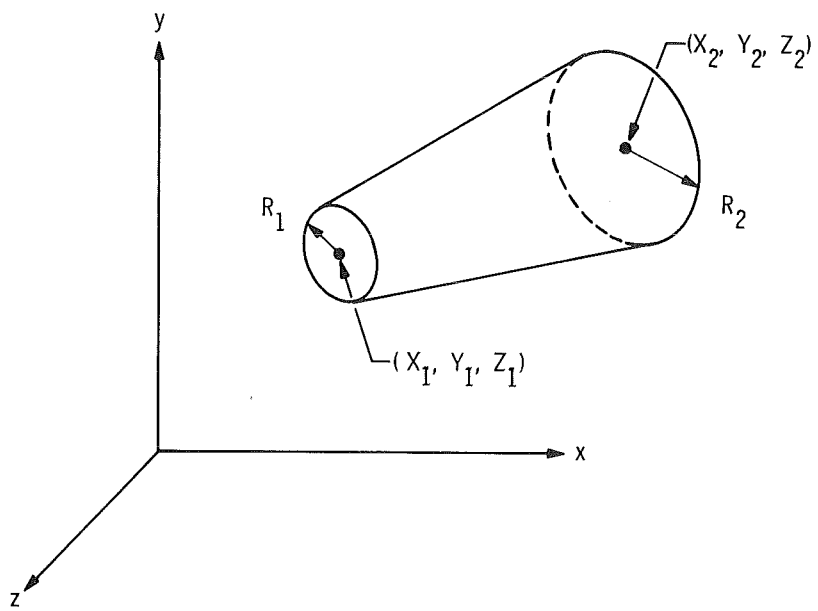


Figure 10. Cone configuration

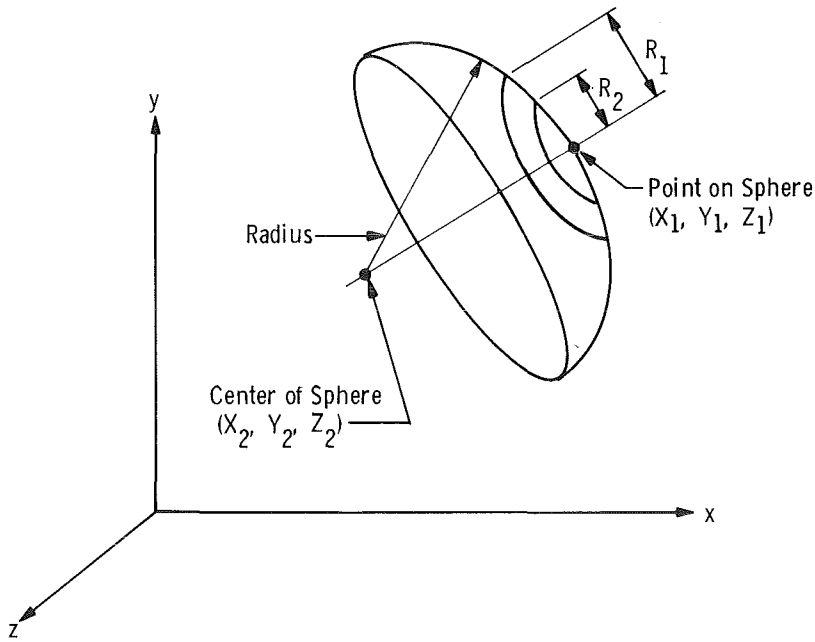


Figure 11. Sphere configuration.

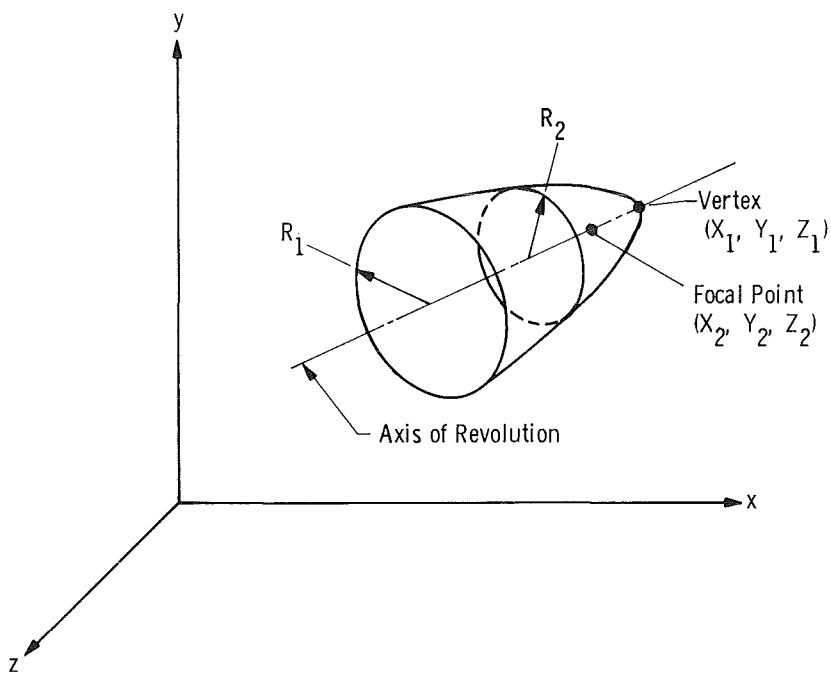


Figure 12. Paraboloid configuration.

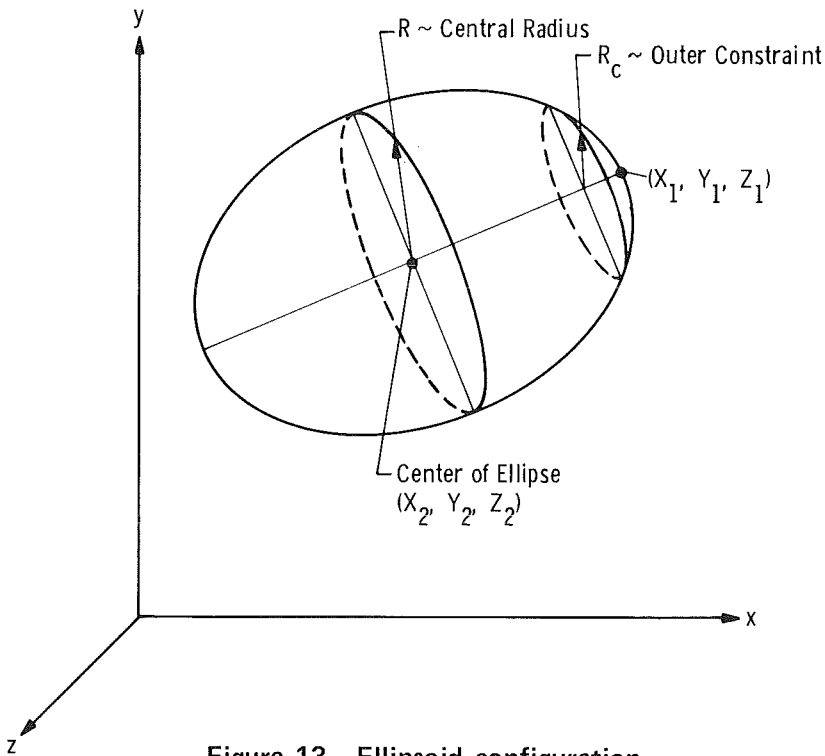


Figure 13. Ellipsoid configuration.

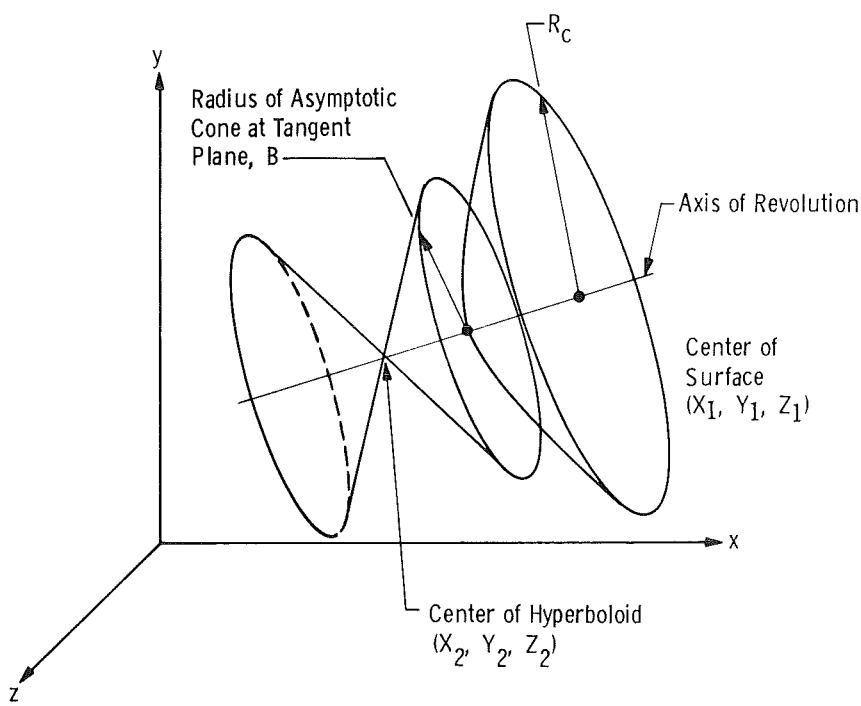


Figure 14. Hyperboloid configuration.

More general surfaces can be input via the variable COEF where

$$COEF\ (J,N) = C_J \qquad J = 1,2, \ldots 10$$

C_J is used in the surface equation, as follows:

$$C_1X^2 + C_2Y^2 + C_3Z^2 + C_xXY + C_5XZ + C_6YZ + C_7X + C_8Y + C_9Z = C_{10} \quad (10)$$

If needed, up to five auxiliary coordinate systems can be defined for referencing the geometric input data. The particular coordinate system for surface N is identified by the variable ICORD(N) = K where K = 0,1...5 (K = 0 is the system coordinate system). The information relating each auxiliary coordinate system to the main system coordinates input through the variable TRFORM(I,J,K). For J = 1 and I = 1,2,3, TRFORM(I,J,K) gives the X,Y, and Z direction cosines of the K^{th} system's X axis; for J = 2, TRFORM(I,J,K) gives the Y-axis direction cosines, and for J = 3 it gives the Z-axis cosines. For J = 4, TRFORM(I,J,K) gives the orgin of the K^{th} system as X, Y, and Z in system coordinates for I = 1,2, and 3, respectively.

Also input through the NMGEOM namelist is IDGREE(N). For any surface input by COEF, IDGREE(N) for that surface must be specified as 2, or it will be computed for the basic surfaces.

The last variable input by means of NMGEOM is LISTOP(I), I = 1,11. LISTOP gives the list of options, a value of 1, which causes printing, and a value of 0, which suppresses that print option. These options for I = 1,11 are as follows:

LISTOP

1. Summary of surface input data
2. Summary of constraint input data
3. Equations of surfaces and constraints
4. Summary of system configuration
5. No longer used
6. Surface property coefficients
7. Spatial maps

8. Radial map and plots
9. Spatial/angular maps
10. Table of energy absorbed by each surface
11. Combined cases computations

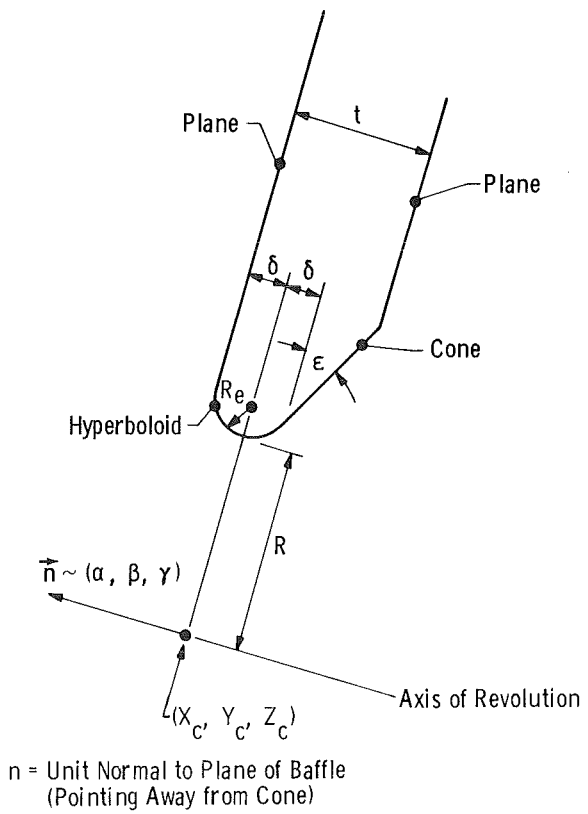


Figure 15. Plane baffle configuration.

3.2 CONSTRAINT INPUTS (NMCNST)

Each surface input through namelist NMGEOM must have defined boundaries or constraints. Several of the standard-type surfaces had standard constraints such as the plane disk or rectangle. Variables input through namelist NMCNST specify the type constraint or define new constraints.

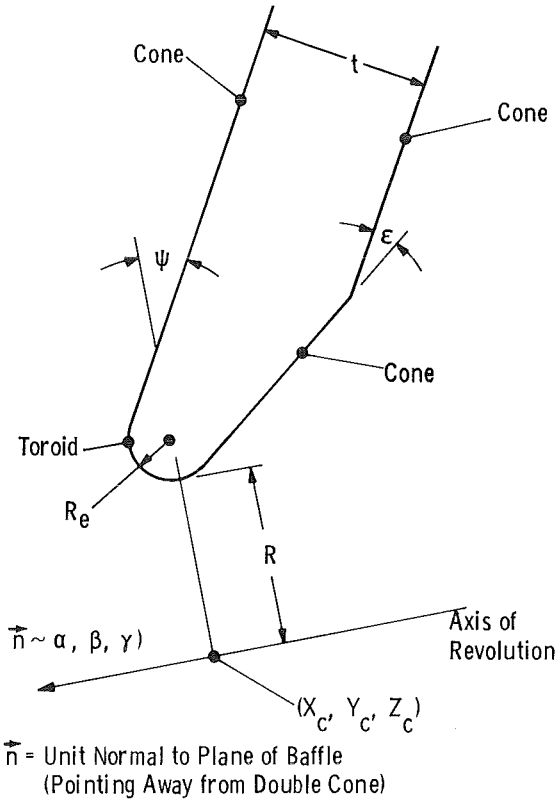


Figure 16. Conical baffle configuration.

The variable NSTRN(N) is equated to the number of constraints of surface N. The number of constraints per surface must be four or less; i.e.,

$$\text{NSTRN(N)} \leq 4$$

Three type constraints can be used. First, the standard as defined in PTLCTR(I,N); second, other boundary surfaces used as defined in namelist NMGEOM; and third, a new constraint surface defined by the parameter PTLCSP(I,M). A plane or conical special constraint surface can be input by means of PTLCSP(I,M) by the same format as used in PTLCTR(I,N) and defined in Table 1. However, no constraints are required for PTLCSP(I,M) since it itself is a constraint. The first special constraint is identified by M = 1, the second by M = 2, etc. There is no necessary relation between the surface number and constraint number.

The special constraint surfaces can be input using the auxiliary coordinate systems that were discussed and could be introduced in NMGEOM. If auxiliary systems are used, they must be identified by the variable ICORSP(M). This variable must be equated to the number of the particular auxiliary system used to input the special constraint.

The variable KSIDSP(I,N) defines the I^{th} constraint of surface N as to type as follows:

1. For an existing surface defined in NMGEOM, set KSIDSP equal to the constraint surface number.
2. For the standard constraint as input by PTLCTR, set KSIDSP equal to zero.
3. For a special constraint defined by PTLCSP(I,M), set KSIDSP equal -M.

One must also specify on which side of a constraint the surface of interest lies. This information is input via the variable KSTRT(J,N) for the J^{th} constraint on surface N, as defined in Table 2.

Table 2. Definition of KSTRT(J,N)

Type Constraint	KSTRT(J,N) =
Plane	1, when surface normal of constraint points away from surface 2, when surface normal points toward surface
Cone, Sphere Paraboloid, Ellipsoid	3, when surface is on concave side of constraint 4, when surface is on convex side of constraint
Hyperboloid	3, when surface is on convex side of constraint 4, when surface is on concave side of constraint
General Surface $F(X,Y,Z) = 0$ where $F = C_1X^2 + C_2Y^2 + C_3Z^2$ $+ C_4XY + C_5XZ + C_6YZ$ $+ C_7X + C_8Y + C_9Z - C_{10}$	3, when $F < 0$ on surface of interest 4, when $F > 0$ on surface of interest

Each special or standard constraint requires computer memory in order to input the constraint surface. Each constraint defined in this way lowers by one the number of surfaces which can be used to define the system boundary. For example, a simple box enclosure, consisting of six plane surfaces, if input via the standard rectangle input with standard

constraints, would require four constraints on each face as well as the six faces. This total would require 30 surfaces, which is the maximum the present version of GUMRAP will handle. This means that each surface is used five times, once as a surface and four times as constraints; this is unnecessarily redundant. If each surface were defined and then used as a constraint, only six out of thirty memory locations would be required. Thus, the way in which the constraints are input becomes very important in utilizing the full capability of the program.

3.3 SURFACE PROPERTY INPUTS (NMCOAT)

Up to 25 different type surfaces can be defined. The definition of each type surface and the identification of each surface type is input through namelist NMCOAT.

The surface properties are input by use of the variable COAT(I,J), which is the I^{th} property of the J^{th}-type surface. The elements of COAT are defined as follows:

COAT(1,J) = the probability that a molecule will be reflected from surface type J according to the reciprocity model;

COAT(2,J) = the probability that a molecule will be reflected from surface type J specularly;

COAT(3,J) = the probability that a molecule will be reflected diffusely with no change in speed;

COAT(4,J) = surface temperature (°K);

COAT(5,J) = the tangential energy accommodation, α_x and α_y;

COAT(6,J) = the normal energy accommodation, α_y.

The last three variables can be omitted if COAT(1,J) = 0.

The variable ICOAT(N) identifies each surface N with a particular type surface J; i.e.,

$$\text{ICOAT(N)} = \text{J}$$

3.4 HEADING AND ISEED

Any number of alphanumeric cards may be input after the end of the NMCOAT namelist. These cards will be printed out twice as headings. The heading cards must be

terminated by the word EXTERNAL (starting in column 1). Next an odd integer called ISEED is input in columns 11 through 20 subject to

$$\text{ISEED} < 2^{31}$$

ISEED is used to start the pseudorandom number sequence generation subroutine used by the Monte Carlo method. For the same value of ISEED the sequence of random numbers produced will be repeated.

3.5 INPUT DATA DEFINING SYSTEM SECTIONS (NMSYST)

As mentioned earlier, a system can be divided into as many as five sections. The definition of these sections is input through the namelist NMSYST. As stated previously, system boundary surfaces are input through namelist NMGEOM, and the constraints are input through namelist NMCNST; in addition, it is necessary to input data to describe on which side of a boundary surface a region or section lies. This is accomplished in this group of inputs.

The surfaces that compose a given section are identified by the variable

$$\text{ISFACE(J,I)} = \text{N}$$

where ISFACE(J,I) describes which system surface, N, defines the J^{th} surface of section I.

The variable KCOEF(J,I) indicates which side of the J^{th} boundary surface of section I the section is on. KCOEF can have values of 0 or 1, as shown in Table 3.

When a system is partitioned into smaller regions or sections, the common surface between adjacent sections will have been input as a boundary surface. The variable ISFTP(I,J) indicates how the various sections are interconnected. This variable is defined as

$$\text{ISFTP(I,J)} = \Delta J$$

where ΔJ is the change in section number in going through the I^{th} surface of section J into an adjacent section, $J + \Delta J$. Notice that ΔJ may be positive or negative. The default value is 0, which indicates a reflection back into the original section (surface I is not an exit).

3.6 INPUT DATA DEFINING MOLECULAR SOURCE (NMEXTL)

The last namelist (NMEXTL) is used to input data concerning the molecular source, entrance and exit apertures, and miscellaneous control parameters.

Table 3. Definition of KCOEF(J,I)

Type Surface	KCOEF(J,I)
Plane	0, when normal of section surface J points away from section I 1, when normal points toward section.
Cone, Sphere, Paraboloid, Ellipsoid	0, when section I is on concave side of section surface J 1, when section is on convex side of surface
Hyperboloid	0, when section I is on convex side of section surface J 1, when section is on concave side of surface
General Surface F(X,Y,Z) = 0	0, when F < 0 in section I 1, when F > 0 in section I

In order for the Monte Carlo ray trace technique to be valid, molecules must be introduced, one at a time, in a realistic fashion into the system. One of the surfaces composing the geometric systems can be designated the entrance by the variable ISENT equated to the surface number of the entrance aperture. The test molecules enter uniformly over the entrance aperture with a direction and divergence given by parameters described below and shown in Fig. 17.

Figure 17 depicts a typical divergent molecular beam passing through a circular entrance aperture. The aperture shown is placed on the X-Y plane of the system coordinates, although this is not necessary. The molecule enters the aperture by the randomized Monte Carlo technique. The entrance aperture can be either circular or rectangular .

The direction of the molecular beam as a whole is defined by the elevation angle, ϕ, which is input via the variable SUNAGD and the azimuthal angle, θ, which is input via the variable SUNAZD. The divergence of the beam (half angle δ) is input via the variable SUNDVD. All angles are in degrees.

The elevation angle, ϕ, is defined as the angle between the beam axis and the Z axis. Notice from Fig. 17 that if $v_z < 0$ then $\phi < 90$ deg. The aximuthal angle θ is the angle between the projection of the beam axis on the X-Y plane and the X axis. Other parameters that are input through the namelist NMEXTL are given in Appendix B.

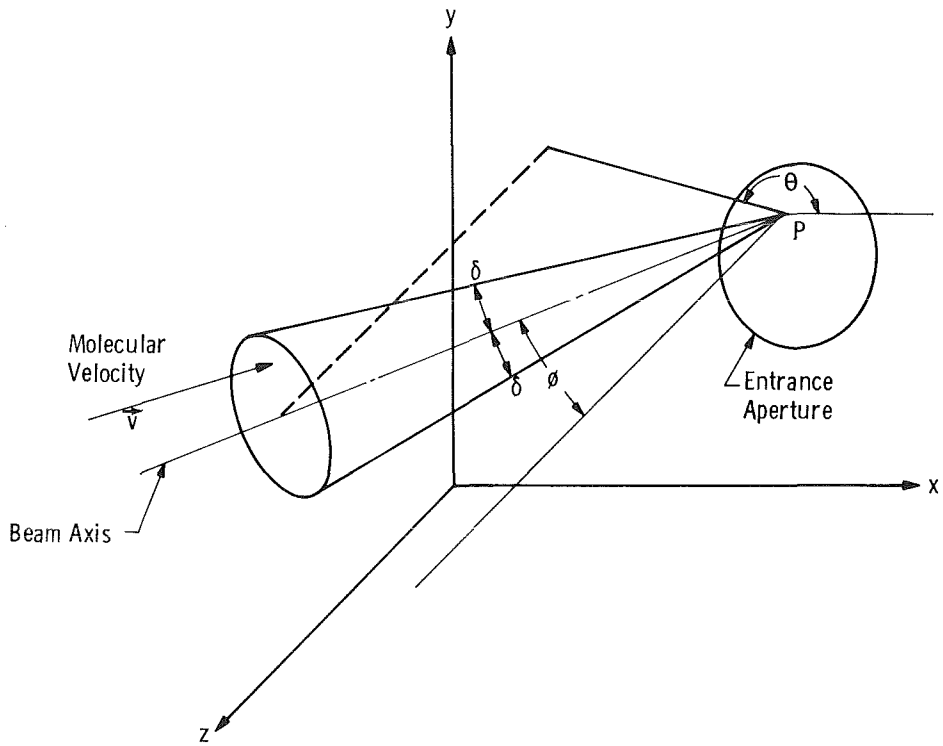


Figure 17. Entrance aperture and molecular beam geometry.

3.7 SAMPLE INPUT DECK

A listing of the card deck necessary to run GUMRAP on an IBM 370/165 computer is shown in Appendix C. Notice that for the namelist input format only the first element in an array name need be given; for example:

PTLCTR(1,8) = 2*.5, 2.222, 0.,etc.

is equivalent to

PTLCTR(1,8) = .5

PTLCTR(2,8) = .5

PTLCTR(3,8) = 2.222

PTLCTR(4,8) = 0.0

etc.

Each namelist starts with an ampersand (&) in colunm 2 followed immediately by the namelist name and then a blank; after this, data items follow on the same or additional cards, separated by commas. Subsequent data cards must start with a blank in column 1, with data starting in column 2. A namelist is terminated by an "ampersand end" (&END), also starting in column 2. The order of data in a given namelist is immaterial. However, the order of the namelists must be followed as given.

4.0 SUMMARY

The General Unwanted Energy Rejection Analysis Program (GUERAP) was used as a basis for a molecular flow analysis program (GUMRAP). The system geometry and Monte Carlo ray trace portion of GUERAP, which was the greater part, was combined with a new Monte Carlo gas-surface interaction program, REFLCT.

It was shown that REFLCT can be used to calculate the resulting conditions for a highly nonequilibrium molecular beam entering an enclosure, and that the Maxwellian velocity distribution as well as the fully accommodated cosine distribution is approached after 10 collisions with the chamber for an accommodation coefficient of 0.9.

All input conditions were defined so that GUMRAP can be run on an IBM 370/165 Computer for complex internal flow geometries.

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8. Kinslow, M. "A Mathematical Description of Gas-Surface Interactions Based on Reciprocity." *AIAA Journal*, Vol. 14, No. 10, October 1976, pp. 1358-1361.

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10. Raeside, D. E. "An Introduction to Monte Carlo Methods." *American Journal of Physics*, Vol. 42, January 1974, pp. 20-26.

APPENDIX A
LISTING OF SUBROUTINE REFLCT

```
      SUBROUTINE REFLCT(V,N)
C
C     GIVEN A MOLECULE WITH VELOCITY VECTOR (V) INCIDENT UPON A SURFACE, N,
C     THIS SUBROUTINE RETURNS IN V THE REFLECTED VELOCITY VECTOR BASED
C     UPON THE RECIPROCIRY RELATION, VELOCITY IN FT/SEC.
C
C     ISEED IN COMMON/SET1/ IS USED IN FUNCTION RN2 TO GENERATE A RANDOM Q.
C
C     WMOLT IN COMMON/SET2/ IS THE GAS MOLECULAR WEIGHT.
C
C     COAT(7,N) AND COAT(8,N) IN COMMON/SET3/ ARE AX AND AY RESPECTIVELY.
C
C     COAT(4,V) IN COMMON/SET3/ IS THE SURFACE TEMPERATURE IN DEGREE K ,TS,
C     OF SURFACE N.
C
C     UGASC IS THE UNIVERSAL GAS CONSTANT IN (FT**2)/(SEC**2)(DEG K)
C
      DIMENSION FT(27,11),FIT(27,5),V(3),A(3)
      COMMON /SET1/ ISEED,KEMIT,KSID,KSTYPE,NSEC,KSEC,IERR,NDIAG,IPOLE,
     1KSSEC,NPOLE,KSECU,IRUN
      COMMON /SET2/ KSIDA,COEF(10,30),KSTRT(4,30),CSTRT(10,4),NQUAR,
     1PTLCTR(11,30),NSTRT(30),IDGREE(30),KSIDSP(4,30),ISTRT(4,30),
     2LSURFC,ICORD(30),TRFORM(3,4,5),LSEC,LSSEC,TCOND,VELINT,WMOLT
      COMMON/SET3/ RAY(6),SURNOR(3),COAT(41,25),E,PHI,THE,RAYP(6),
     1ESAVE,ETHERM(30),IEMODL(25),LISTOP(11),ICOAT(30)
      DATA UGASC/89523./
      EQUIVALENCE (FIT(1,1),FT(1,7))
      DATA FT/
     2 .0260, .1427, .2023, .2489, .2888, .3246, .4032, .4724, .5364,
     3 .5972, .6563, .7147, .7732, .8326, .8936, .9572,1.0246,1.0973,
     41.1774,1.2686,1.3774,1.5174,1.5892,1.6773,1.7941,1.9779,2.4930,
     5-.0400, .0713, .1325, .1804, .2214, .2582, .3390, .4101, .4759,
     6 .5384, .5992, .6592, .7193, .7803, .8430, .9083, .9775,1.0521,
     71.1344,1.2280,1.3396,1.4833,1.5570,1.6473,1.7669,1.9552,2.4823,
     8-.1030, .0056, .0688, .1184, .1609, .1990, .2825, .3562, .4242,
     9 .4888, .5516, .6136, .6756, .7386, .8032, .8706, .9420,1.0188,
     A1.1035,1.1998,1.3145,1.4619,1.5375,1.6300,1.7525,1.9449,2.4821,
     B-.1840,-.0637, .0023, .0542, .0987, .1385, .2257, .3025, .3734,
     C .4407, .5060, .5705, .6349, .7002, .7673, .8371, .9109, .9903,
     D1.0777,1.1769,1.2949,1.4462,1.5236,1.6183,1.7435,1.9397,2.4850,
     E-.2670,-.1412,-.0708,-.0158, .0313, .0734, .1655, .2466, .3213,
     F .3921, .4607, .5282, .5956, .6638, .7337, .8064, .8830, .9652,
     G1.0556,1.1579,1.2792,1.4344,1.5136,1.6103,1.7379,1.9374,2.4895,
     H-.3690,-.2317,-.1551,-.0956,-.0447, .0007, .1000, .1869, .2667,
     I .3421, .4149, .4863, .5574, .6291, .7023, .7782, .8579, .9432,
     J1.0367,1.1422,1.2668,1.4256,1.5064,1.6050,1.7347,1.9371,2.4948/
      DATA FIT/
     K-.4890,-.3424,-.2564,-.1896,-.1327,-.0821, .0276, .1229, .2097,
     L .2912, .3694, .4456, .5211, .5967, .6737, .7530, .8360, .9244,
     M1.0209,1.1294,1.2571,1.4193,1.5015,1.6016,1.7333,1.9381,2.5006,
```

```
     N=.6740,-.4854,-.3815,-.3020,-.2351,-.1762,-.0505, .0567, .1528,
     O .2419, .3263, .4079, .4881, .5679, .6485, .7312, .8173, .9087,
     P1.0080,1.1192,1.2496,1.4147,1.4982,1.5997,1.7330,1.9400,2.5069,
     Q-.9430,-.6725,-.5312,-.4284,-.3449,-.2734,-.1259,-.0047, .1015,
     R .1982, .2888, .3754, .4597, .5432, .6271, .7127, .8015, .8954,
     S .9971,1.1107,1.2435,1.4112,1.4960,1.5988,1.7336,1.9427,2.5140,
     T-1.3420,-.8577,-.0619,-.5330,-.4335,-.3510,-.1861,-.0542,.0595,
     U .1618, .2570, .3474, .4351, .5215, .6080, .6961, .7872, .8833,
     V .9872,1.1031,1.2382,1.4085,1.4944,1.5986,1.7350,1.9463,2.5225,
     W-1.5370,-.9522,-.7379,-.5994,-.4935,-.4062,-.2329,-.0951, .0231,
     X .1292, .2275, .3209, .4111, .5000, .5889, .6791, .7725, .8708,
     Y .9769,1.0951,1.2329,1.4062,1.4935,1.5994,1.7379,1.9522,2.5355/
      WM = WMOLT
      TS = COAT(4,N)
      VW=SQRT(2.*UGASC*TS/WM)
      A(1) = COAT(7,N)
      A(2) = COAT(8,N)
      A(3) = COAT(7,N)
      DO 4 K=1,3
      S=V(K)/VW
      R = SQRT(A(K)**2 - 1.0)*S
      CALL RN2(ISEED,Q)
      FR=1.
      IF (K.EQ.2) FR=R*R/(.5+R*R)
      IF (Q.LE.0.1) GO TO 1
      IF (Q.GT.0.9) GO TO 2
      IX=20*Q
      I=IX +4
      X=20.*Q-IX
      GO TO 3
    1 IX=50*Q
      I=IX+1
      X=50.*Q-IX
      GO TO 3
    2 IX=50*Q
      I=IX-23
      X=50.*Q-IX
    3 IF(FR.EQ.1.0) GO TO 5
      IY=10*FR
      J=IY +1
      Y=10.*FR-IY
      FTO=(1.-Y)*((1.-X)*FT(I,J)+X*FT(I+1,J))
     $+Y*((1.-X)*FT(I,J+1)+X*FT(I+1,J+1))
      T = FTO + (R*R/(0.5 + R))
      GO TO 6
    5 FTO= (1.-X)*FT(I,11)+X*FT(I+1,11)
      T=FTO-.5+R
    6 V(K) = T*VW/A(K)
    4 CONTINUE
      RETURN
      END
```

APPENDIX B
LISTING, DEFINITION, AND DEFAULT VALUES OF INPUT VARIABLES

NAMELIST — NMEGEOM

Variable	Definition	Default Value
IPLANE(I)	Surface number of the I^{th} plane.	0
ICONE(I)	Surface number of the I^{th} cone.	0
ISPHER(I)	Surface number of the I^{th} sphere.	0
IPARAB(I)	Surface number of the I^{th} paraboloid.	0
IELPS(I)	Surface number of the I^{th} ellipsoid.	0
IHYPB(I)	Surface number of the I^{th} hyperboloid.	0
IBAFF(I)	Surface number of the I^{th} baffle.	0
PTLCTR(J,N)	J^{th} parameter describing standard surface N (see Table 1).	0
COEF(J,N)	Coefficient, C_J, for special surface N defined by Eq. (32).	0
RKNIFE	R_e (see Figs. 15 and 16).	0
TBAFF	t, thickness of baffle (see Figs. 15 and 16).	0
DBAFF	δ (see Fig. 15).	0
ABAFFD	ϵ, baffle blade angle (see Figs. 15 and 16).	0
IDGREE(N)	Degree of equation for surface N = 2 for special surface.	Computed for standard surfaces
TRFORM(I,J,K)	Rotation matrix and origin of auxiliary coordinate system K (see Section 3.1).	
ICORD(N)	= K, coordinate system used for input data of surface N.	0 (System coordinates)
LISTOP(I)	= 1 for any option wanted (see Section 3.1).	0 (No output)

NAMELIST — NMCNST

Variable	Definition	Default Value
NSTRT(N)	Number of constraints on surface (N), ≤ 4, must be entered for all surfaces.	0
KSIDSP(I,N)	Definition of the I^{th} constraint type for surface N (see Section 3.2).	0 (Standard defined by PTLCTR)
KSTRT(I,N)	Type of the I^{th} constraint of surface N (see Table 2).	0
PTLCSP(I,N)	Special I^{th} constraint for surface N (plane or cone) by same format as PTLCTR (Table 1).	0
ICORSP(M)	= K, coordinate system used for input data of special constraint, M.	0 (System coordinates)

NAMELIST — NMCOAT

Variable	Definition	Default Value
COAT(I,J)	I^{th} properties of surface type J (see Section 3.3).	0
ICOAT(N)	= J, surface type of surface N.	0

After NMCOAT, cards containing a title to be printed on the output can be included. Next the word EXTERNAL starting in column 1 must be included, followed by the value of ISEED (See Section 3.4).

NAMELIST — NMSYST

Variable	Definition	Default Value
ISFACE(J,I)	= N, the surface number of the J^{th} surface of Section I.	0
KCOEF(J,I)	coefficient indicating which side of the J^{th} surface section I is on (see Table 3).	0
ISFTP(J,I)	= ΔJ, change in section number for molecules exiting through surface I of Section J; may be + or -.	0

NAMELIST — NMESTL

Variable	Definition	Default Value
NSEC	Number of sections in the system ≤ 5.	1
LEMIT	Number of molecules that enter the system.	0
LRFN	Limit on number of molecular surface encounters.	20
ISEEDP	After every ISEEDP molecules enter the system, the value of ISEED is printed out; these ISEED values can be used to continue or repeat the computation.	100
NPRINT	Limit on number of molecules for which the ray tracing will be printed in arriving at the exit aperture.	200
RMAP	Radius of the molecular distribution map at the exit aperture.	0
KPRINT	Input for printing ray trace history of rays that did not reach the exit aperture. Set any positive integer and print will occur after first KPRINT molecules. If $=0$ no such printout will occur.	0
ISEXT	Exit aperture surface number.	
JPRINT	Number of molecules with one line summary printout.	1
SUNAGD	Elevation angle of incident beam, ϕ (degrees); see Fig. 17.	0
SUNAZD	Azimuth angle of incident beam, θ (degrees); see Fig. 17.	0
SUNDVD	Divergence angle of incident beam, δ (degrees); see Fig. 17.	0
ISENT	Entrance aperture surface number.	-

NAMELIST — NMESTL (Concluded)

Variable	Definition	Default Value
IENTTP	= 0 for circular entrance, = 1 for rectangular entrance.	0
IESTTP	= 0 for circular exit, = 1 for rectangular exit.	0
KSECST	Section number in which molecules originate.	1
ICSENT	Coordinate system for the entrance section.	0
VELINT	Initial velocity of molecules entering system (ft/sec).	1000
TCOND	Condensation temperature of molecules (°K).	77.
WMOLT	Molecular weight of molecules.	28.

APPENDIX C
SAMPLE GUMRAP INPUT DECK FOR IBM 370/165

```
/*PRIORITY      5
//ASB05919    JOB           (ARO,
//                VRV00203,01,V32K-15A),02489KINSLOW,MSGLEVEL=1,
//    CLASS=X,TIME=(,15),REGION=190K
//      EXEC FORTEPDS,PGMNO=VRV00203
//GO.FT05F001 DD UNIT=WORK,SPACE=(CYL,(9,1),RLSE,,ROUND),
//       DCB=(RECFM=VBS,LRECL=84,BLKSIZE=844)
//GO.FT04F001 DD *
 &NMGEOM
 IPLANE(1)=1,8,11,
 PTLCTR(1,1)=.5,.5,0.,0.,0.,1.,1.,1.,1.,0.,0.,
 COEF(1,2)=7*0.,1.,-1.,1.,
 COEF(1,3)=7*0.,1.,-1.,0.,
 COEF(1,4)=6*0.,1.,0.,0.,0.,
 COEF(1,5)=6*0.,1.,0.,0.,1.,
 COEF(1,6)=7*0.,1.,1.,3.222,
 COEF(1,7)=7*0.,1.,1.,2.222,
 PTLCTR(1,8)=.5,.5,2.222,0.,0.,-1.,1.,1.,1.,0.,0.,
 COEF(1,9)=6*0.,1.,0.,0.,0.,
 COEF(1,10)=6*0.,1.,0.,0.,1.,
 PTLCTR(1,11)=.5,1.6111,1.111,0.,0.,1.,1.,1.,1.,0.,0.,
 IDGREE(1)=1,6*2,1,2,2,1,
 LISTOP(1)=1,1,1,1,1,1,1,1,1,1,0,
 &END
 &NMCNST
 NSTRT(1)=11*4,
 KSIDSP(1,1)=2,3,4,5,
 KSIDSP(1,2)=1,4,5,6,
 KSIDSP(1,3)=1,4,5,7,
 KSIDSP(1,4)=1,2,3,11,
 KSIDSP(1,5)=1,2,3,11,
 KSIDSP(1,6)=8,9,10,2,
 KSIDSP(1,7)=8,9,10,3,
 KSIDSP(1,8)=6,7,9,10,
 KSIDSP(1,9)=6,7,8,11,
 KSIDSP(1,10)=6,7,8,11,
 KSIDSP(1,11)=2,3,4,5,
 KSTRT(1,1)=1,2,2,1,
 KSTRT(1,2)=2,2,1,1,
 KSTRT(1,3)=2,2,1,1,
 KSTRT(1,4)=2,1,2,1,
 KSTRT(1,5)=2,1,2,1,
 KSTRT(1,6)=2,2,1,1,
 KSTRT(1,7)=2,2,1,1,
 KSTRT(1,8)=1,2,2,1,
 KSTRT(1,9)=1,2,2,2,
 KSTRT(1,10)=1,2,2,2,
 KSTRT(1,11)=1,2,2,1,
 &END
```

```
 &NMCOAT
 COAT(1,1)=1.0,0.,0.,300.,0.5,0.5,
 COAT(1,2)=0.,1.0,0.0,
 ICOAT(1)=2,1,1,2,2,1,1,2,2,2,2,
 &END
 TEST CASE FOR 1X1X1 CHEVRON BAFFLE DESIGN
 PROJECT NO. V32K-15A,GUMRAP MOLECULAR ANALYSIS
 KINSLOW,AUGUST 1979.
EXTERNAL
             13131313
 &NMSYST
 ISFACE(1,1)=1,2,3,4,5,11,
 ISFACE(1,2)=11,6,7,8,9,10,
 KCOEF(1,1)=1,0,1,1,0,0,
 KCOEF(1,2)=1,0,1,1,1,0,
 ISFTP(1,1)=5*0,1,
 ISFTP(1,2)=-1,
 &END
 &NMEXTL
 NSEC=2,
 LEMIT=50,
 RMAP=.5,
 LRFN=40,
 KPRINT=1,
 ISEXT=8,
 JPRINT=10,
 NPRINT=50,
 SUNAGD=180.,
 SUNDVD=90.,
 VELINT=20000.,
 WMOLT=40.,
 ISENT=1,
 IENTTP=1,
 IEXTTP=1,
 &END
//GO.FT04F002 DD *
/*
/*
```

NOMENCLATURE

A_x, A_y, etc.	Constant ≥ related to α_x, α_y by Eq. (5)
N	Number of surface collisions in Section 2.3, surface number in Section 3
$\vec{n}$	Unit normal vector with direction cosines (α,β,γ)
$P(\vec{v}',\vec{v})$	Scattering kernel
$P_x(v_x',v_x)$, $P_y(v_y',v_y)$, etc.	Scattering kernel in corresponding coordinate direction
R	Gas constant per unit mass, radius in Figs. 13, 15, 16
R_1,R_2	Radii
Re	See Fig. 16
R_x	$\sqrt{A_x^2 - 1}\, S_x'$
R_y	$\sqrt{A_y^2 - 1}\, S_y'$
S,S_x', etc.	Dimensionless velocity, $v/\sqrt{2RT_s}$, $v_x'/\sqrt{2RT_s}$, etc.
T_s	Wall or surface temperature
T_x	A_xS_x
T_y	A_yS_y
t	See Fig. 15
$\vec{v}$	Reflected molecular velocity
$\vec{v}'$	Incident molecular velocity
v_x,v_y', etc.	Velocity component in corresponding coordinate
X, Y, Z	Coordinate axis (see Fig. 1)
α	Thermal accommodation coefficient
α_x, α_y, etc.	Accomodation coefficient in corresponding coordinate direction

δ	See Fig. 15 or Fig. 17
ϵ	See Fig. 15 or Fig. 16
θ,ϕ	See Fig. 1 or Fig. 17
ψ	See Fig. 16